

CP-FTMW SPECTROSCOPY OF 2-CYANOACETIC ACID

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2-Cyanoacetic acid (m.p. 67-73 °C), a molecule with astrochemical significance and structural similarities to glycine^a has been transferred into the gas phase by heating and supersonic expansion. Possible conformational relaxation paths were explored by using different buffer gases such as neon, argon, and helium. Rotational constants were found using chirped-pulse Fourier transform microwave spectroscopy (CP-FTMW). 2-Cyanoacetic acid possesses one ¹⁴N nucleus with a nuclear quadrupole moment, giving rise to a complex hyperfine structure. To assist with spectral fitting, Autofit^b was used. One stable conformer of the monomer and its complex with a water molecule have been identified on the basis of the experimental rotational constants in conjunction with DFT and *ab initio* predictions.

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